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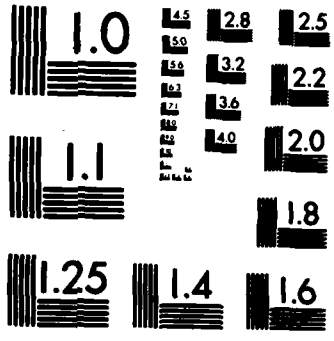

Department of Physics and Astronomy
University of Maryland
College Park, MD 20742

"Theory and Calculations of the Electronic Structure of Solids Having Directional Bonding"

Final Report
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(1) The Energy Band Gap in Semiconductors and Insulators:

Probably the most important single parameter of a semiconductor is its energy gap. It has been established that the density functional theory, which yields an excellent description of the ground state properties of solids, under-estimates the band gaps in semiconductors and insulators by 30% to 50%. We have developed a general approach to the calculation of quasi-particle excitations. Our main contribution lies in recognizing that when there is a gap, the screening of the Coulomb potential is not nearly as large as it is with no gap. This effect was incorporated in a computationally feasible way, and the resulting self-energy for a prototype semiconductor (Si) and a wide gap insulator (diamond) is much larger, and in nice agreement with experiment. For the Physical Review Letter announcing this result, we received the 1983 research and publication award in our division at the Naval Research Laboratory. A longer paper has just appeared. These results and its extension will be presented at the 1985 APS March meeting symposium.

(2) Structural Properties of Solids

It has recently been established that the local spin density approximation (LSDA) within the density functional theory can provide an accurate theoretical estimates of static structural properties, phonon spectra, crystal stability, and pressure-induced phase transformations in solids. Under the current contract we have calculated the total energies

as a function of volume, using the full potential linearized augmented plane wave (LAPW) method, for a number of different systems. Among our major results, we found that the experimental equilibrium lattice constant and bulk modulus are reproduced to better than 1% and 5%, respectively, for covalent semiconductors (Si and GaAs) and metallic compound (NbC). Recently, Pickett et al. predicted that B1-structure MoN would be a high T_c superconductor with a $T_c \approx 30°K$. Given the possibility of such a dramatic increase in T_c, a number of experimental efforts, so far unsuccessful, to form stoichiometric B1-structure MoN have been undertaken. We are now studying the difference in total energy between hexagonal and B1-Structure of MoN in order to determine the transition pressure needed to lock-in the B1 structure, which should be a valuable guide to the experimental efforts.

(3) Magnetic and Structural Ordering in Iron:

The accuracy of LSDA in describing the magnetic and structural ordering in 3-d transition metals is not as good as that of non-magnetic materials. In a recent study we have calculated the total energy of non-magnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM) states for both bcc and fcc phases of iron for a range of atomic volumes near equilibrium. The FM state was found to have the lowest energy in the bcc case while the AFM state is almost degenerate with the NM state in the fcc case. Surprisingly, the latter lies lower in energy than the former, which is the actual ground state of iron at zero temperature. The failure to predict the proper ground state of iron indicates a fundamental difficulty in the LSDA for describing the magnetic interaction in 3-d transition metals. Possible ways of improving LSDA is being investigated.

(4) Anomlalous Quantum Hall Effects.

Recent discovery of the anomalous quantum hall effects have excited enormous interest. We have calculated the wave functions and correlation energies of two-dimensional electrons in a strong magnetic field based on the density functional theory. For an appropriate density functional, we were able to get good agreement with exact numerical results based on finite size systems.

So far our work has resulted in one invited paper, fourteen contributed papers, and seven extensive manuscripts which are enclosed.

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